A STUDY OF '1'1 IE LINE PROFILE OF 11L YMAN-β FROM DISSOCIATIVE EXCITATION 01"1\$

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ABSTRACT

A high-resolu ion ultraviolet (uv) spectrometer was employed for measurement of the HLyman-β (}1 Lβ) emission Doppler line profile a t 1025.7 Å from dissociative excitation of H₂ by electron impact. Analysis of the (ice.onvolvcci line profile reveals the existence of a narrow central peak, less than 30 mÅ full-width-half-maximum (FWHM) and a broad pedestal base shout 260 mÅ FWIIM. Analysis of the red wing of the line profile is complicated by a group of Werner and I syman rotational lines 160 to 2 2() mÅ from line center. Analysis of the blue wing of the line profile gives the kinetic energy distribution. '1'here are two main kinetic energy components to the H(3p) distribution: 1) a slow distribution with a peak value near O CV from singly excited states and 2) a fast distribution with peak contribution near 7 eV f r o m doubly excited states. Using two different techniques, the absolute cross section of 11 Lβ is found 10 be 3.28 ± 0.80 x 10⁻¹⁹ cm² at 100 eV c ectron impact energy. The exper mental cross section and line profile results can be compared to previous studies of Ha (6563.7 Å) for principal quantum number n=3 and of L α (121 5.7 Å) for n=2.

PACS CLASSIFICATION: 34.80.Gs (ELECTRON SCATTERING-MOLECULAR DISSOCIATION), 33.50Dq (Mel_ECULAR SPECTRA - FLUORESCENCE

INTRODUCTION

For many years high resolution studies in the visible region of the spectrum have been carried out on the Balmer series {principal q u an t um 1111111ber, n=3, 4 and 5 excited states) of H produced by dissociative excitation of H₂ upon electron impact. For each principal quantum number, two major sets of kinetic energy distributions were found, corresponding to the "slow" and "fast" distributions with typical kinetic energies of near O Cv, respectively. The principal architects of these cV and 4-10 measurements were Ogawa and co-workers. 1-3 They have carefully shown that the two kinetic energy distributions reflect effects of dissociation from singly excited bound states (slow component) and from repulsive doubly excited states (fast component). Recently, we have begun high resolution studies of the Lyman series of 11 from dissociative excitation of H₂, 4,5 utilizing a high resolution 3-meter vacuum ultraviolet (vuv) spectrometer with a resolving power of greater than 50000. ('We reported the first measurement of the HLyman-α (HLα) emission] Doppler profile f rom impact. Analysis of the dissociative excitation 11, by electron of deconvolved line profile revealed the existence of a narrow central peak of 40 + 4 mÅ FWIIM and a broad pedestal base about ?40 mÅ wide FWHM. Slow II(2p) atoms with peak energy near 80 meV produce the peak profile, which is nearly independent of impact energy. The wings of 11 Lα arise from dissociative excitation of a series of doubly excited Q₁ and Q₂ states, which define the core orbitals. The energy distribution of the fast atoms **shows** a peak at about 4 cV. in this work we extend the measurements to he 3p state and compare our results to line profile studies of Hα. The Hα inc profile shows a characteristic narrow central peak (-300 mÅFWHM) from the slow component and a broad wing (-1.8 ÅFWH M) from the fast Component in the optical region. Since the Doppler displacement is proportional to wavelength, six times narrower line profiles can be expected in the vacuum ultraviolet (vnv) spectral region for the L ym a n series.

l is also a goa of this study to directly measure the absolute cross section for HL β at 100 Cv for completely modeling the 11_2 vacuum ultraviolet spectrum (vuv) for both calibration and astronomy purposes. Once before, in 1984 we have applied published H α absolute cross section results to a low resolution H₂ Vuv spectrum from our laboratory to determine the absolute HL β absolute cross section. ~

The most important application of the Lyman series line profiles is the opportunity to study and distinguish the emission spectrum of hydrogen from its molecular and atomic orms. The advent of high

resolution spacecraft such as the Hubble Space Telescope, equipped with the Goddard High Resolution Spectrograph and the planned astrophysical extreme ultraviolet observatories have lead to the measurement of the H L α line profile in both the auroral zones and the day glow. 11 L α Jine profile wings extending to ±1 Å have been measured in the aurora by HST and line core widths of greater than J 40 mÅ have been observed by IUE. 9,10 The primary cause of the dayglow is resonant scattering of solar emission with a broad Jine profile from multiple scattering. The main cause of the aur ora is primary particle bombardment by electrons, protons and heavier ions followed by secondary electron excitation of the. J yman series. The and Werner band emission large amount of Lyman ensures that dissociative excitation of H₂ is an important process.

EXPERIMENTAL

The experimental system has been described by J in et al.⁶ in brief, the experimental system consists of a high-resolution 3-meter uv spectrometer in tandem with an electron impact collision chamber. For the Lβ Jine profile, a resolving power of 27,000 is achieved by operating the spectrometer in second order. The 11 Lα line profile has been previous by

reported^{4,5} and was measured in third order at a resolving power of 50,()()0. 'he line shapes were measured with experimental conditions that ensure 1 nearity of signal with electron beam current and background gas pressure, in this study the line profile spectra were measured in the crossed beam mode; and the one. low resolution HLB excitation function was obtained in the static gas mode. The operating conditions for the collision chamber included an electron beam current of 130 µA and an H₂ gas pressure of 2.3 x 10'4 torr. The electron -impact -induced -fluorescence line profiles of HLα and HLβ at 100 CV impact energy are shown in Fig. 1, along with the instrumental slit function of the spectrometer in second order. It is found that the H . \beta line profile has a red wing that is blended by three moderately strong Lyman (L) and Werner (W) rotational lines, detailed in 'J'able 1 among other rotational lines in the neighborhood of the red wing of IILβ. One of the three strong incs is the L1(6,0)Q resonance line, lying furthest from HLB line center. The closest, the W 1 (5,3)Q rotational line lies 163 mÅ from HLB line, center. Wc estimate the extent of the red wing by reflecting he blue wing about line center, It is shown as a dashed line in Fig. 1. The major wing of the H 1\$ line profile extends 150 mÅ from line center. A very weak secondary pedestal wing extends to 175 mÅ from line center. By comparison the H Lα wing extends 1 40 m Å

(reported FWHM = 240 mÅ) from line center.^{4,5} The Doppler wavelength shift is proportional to the rest wavelength. Much greater kinetic energies are released during n=3p dissociation than for n=2) (Dissociation to account for the broader HL β line profile.

The weak signal from HL\$\beta\$ in third order prompted the second order study. Yet note the line core FWHM is nearly (40 m\$\beta\$ vs 38 m\$\beta\$) at the limit of the second order slit function. It is slightly narrower than the third order line core profile from HL\$\alpha\$ even though the HL\$\alpha\$ slit function was a narrow 24 m\$\beta\$ that is indicated in Fig. 1. For this reason it will not be possible 10 accurately determine the slow atom distribution function as we certain which were able to do for HL\$\alpha\$.

11 Lβ CROSS SECTION AT 100eV

The first step in our comparative study of $11 \text{ L}\alpha$ and $11 \text{ L}\beta$ was to measure the absolute cross section of $11 \text{ L}\beta$ at 100 cV. We can find the cross section by two methods. One method relies on the absolute cross section of $11 \text{ L}\alpha$ al 10(cV), together with a relative calibration of $11 \text{ L}\alpha$ and $11 \text{ L}\beta$ line intensities, and the other method uses the absolute cross sections of the three major 1.8 W features in the red wing of $1.4 \text{ L}\beta$.

For the first method, the cross section of $1 L\alpha$ has been measured to be '7.3 x 10^{-18} cm² at 100 eV. The relative calibration in the vuv at 100 cV, using the 1 l₂ "many line" spectrum, has been described in fine structure. 6,11 The two step process involved: 1) measuring the HLβ to }1 I.α intensity ratio at 100 CV and 2) determining the relative calibration between 1025 Å and 121.6 Å. The wavelength calibration was performed in second order using the synthetic vuv line intensities of Liu et al.6 as the experimental low resolution convolved to the same resolution spectrum. Approximately sixteen continuous 2S Å wide spectral regions resolution provided a smooth second order calibration curve between 900 and 1300 Å. A typical first order FUV calibration curve is shown in Liu c t By applying this first method, the ratio of cross sections was al." determined to be Q(H L β)/Q(H L α) = 0.0412 at 100 eV. Q(H L β) is 3.01 ± 0.75 $\times 10^{-19} \text{ cm}^2$.

The second method gave an independent evaluation of the cross section. It is also a method that is free of instrument calibration. We have recently measured for the first time the L&W fine structure direct cross section energy dependence from O - 1 keV (Liu et al., unpublished). Using the oscillator strengths of Abgrall et al. 12 14, we are able to place on a nabsolute scale the cross section for every rotational line at 100 Cv. The

three strong 1. & W rotational lines found in the red wing of the HL β line are shown in 'l-able 1, along with corresponding intensities. The 1 (6,0)1'L rotational line required a 40% correction for optical depth at t h c measurement pressure of 2.3 x 10-4 torrand the path length of foreground gas of 11.05 cm. The fractional 1. & W area of the total blended L β + 1, & W feature in Fig.1 is 42.4%. The ratio of Q(L β)/Q(L&W) is 1.36. At 100 cV, w c find the cross section of HL β to be 3.43 ± 0.8S x 10 ¹⁹ cm². "1'he average cross section of HL β at 100 CV based on these two methods is 3.22 ± 0.80 x 10^{-19} cm². The total cross section of the blended feature in Fig.1 is 5.69 ± 1.40 x 10^{-19} cm²

KINETICENERGY DISTRILIJ'1'10N OF FAST PRODUCTS

The determination of the kinetic energy distribution of the products is a two-step process that we have described in the previous paper on H $1.\alpha.^{4.5}$ The resolution of the experiment is not sufficient to recover the slow distribution of 11(3p) atoms. However, the width of the wings is broad with respect to the instrument slit function. On this basis it should be possible to locate the peak of the kinetic energy distribution function of fast 11(3p) and estimate the shape of the distribution function. The measured line profile is the convolution of the true line profile and the instrumental slit

function. Expressed mathematically the measured line profile, $I(\lambda)$, is given by the convolution integral

$$I(\lambda) = \int T(\lambda') A(\lambda - \lambda') d\lambda', (1)$$

where $T(\lambda')$ is the true line profile at wavelength λ' and $A(\lambda-\lambda')$ is the instrumental response function. In the transform domain the convolution becomes a simple product,

$$I_{T}(s) = "I'.,.(s) A.,.(s),$$
 (2)

where 13., T_T , and A_T are the FFT of I, T and A, respectively and s is measured in inverse wavelength. Optimal Wiener filtering of the measured signal, 1, was performed, since it includes a small noise component. SigJ]al-to-noise ratio (S/N) is greater than 40 for all line profiles. The FFT of '1' is given by,

$$T_{\tau}(s) = L(s) F_{\tau}(s) / A_{\tau}(s)$$
, (3)

where $F(\lambda)$ is the optimal filter. We selected a $cosine^{40}(s)$ to remove high frequency noise from the ratio of n/Al.. We show in 1 fig. 2 the inverse IFT (FFT-1) of $T_T(s)$ for the 100 CV line profiles of H La and H Lβ compared to the wavelength scaled Hα results of Freund et al. ¹⁶ and Higo et al. ² The Lβ feature arises from a single multiplet corresponding to the transition 1 s-3p. However the Hα feature—consists of three multiplets from the transitions 2s-3p, 2p-3s and 2p-3d. Only the first Hα multiplet (2 s-3p)

shares the Same u_{pper} level. For that $H\alpha$ multiplet the line profile would be identical to $L\beta$ when scaled in wavelength by the factor 1025.7Å /6563.7Å, according to the Doppler principle. In the comparison in Fig. 2, we have assumed that all three multiples produce the same line profile. This is plausible since their 3ℓ dissociation asymptotes are degenerate.

The first interpretation from Fig. 2 comes from a comparison of the 100 CV line profiles of H Lα and HLβ. The wings of f Lβ line profile arc broader and more intense than H Lα. The FWHM of H α is 240 mÅ while the HLB line profile has a FWHM of 260 mÅ. The ratio of the two FWHM $(L\beta/L\alpha)$ is a modest 1.08. This ratio can be used to find the ratio of the average kinetic energy for fast H(3p) and H(2p) atoms. The ratio is mad c larger by an additional factor of 1 .41 when converting the Doppler shifts to an equivalent translational energy. More details on the energy dependence distribution are discussed below. As described earlier, we were only of the able to measure an unblended line profile for the blue wing of HLB. We have assumed the red wing is identical. Since the IIa line is slightly asymmetric, the same can be expected to be true of HLβ. The comparison of the IIL β line profile with the two published $H\alpha$ line profiles is in quite good agreement with the results of Higo et al.² and verified recently b y Ogawa et al.3 The comparison with Freund et al. 16 is quite poor. Those

authors have pointed out that their H α line profiles were flawed by spectrometer aberrations. Note the H α line profile of Higo et al.² and the L β line profile indicate the appearance of a weak secondary wing extending to nearly 200 mÅ from L β line center. The initial indication from our data is that the line core of H L α is broader than for HL β , in Fig. 1 at the lower resolution afforded by second order for H 1 β we find a narrower line than for 11 L α . This result can be attributed to the energy scale relating to the processes for production of slow H(2p) atoms from direct excitation, cascade and predissociation, particularly the later. 4.5.17.18 We place an upper limit of 30 mÅ on the FWHM of HL β compared to our previously reported value of 40 mÅ for H 1 α .

For the 100 eV line profile The kinetic energy distribution of the fragments, P(E), is given by

$$P(E) = k(dT/d\lambda)$$
, (4)

where k is a multiplicative constant .19 With this approach, the $100 \, eV$ electron impact line profiles for H L α and H L β in Fig. 2 were differentiated. The combined kinetic energy distributions of the fast and slow H(2p) and H(3p) fragments are shown in Fig. 3 for the blue wing of H L α and H L β of Fig. 3. The results for the H(3p) atom distribution show a peak kinetic energy at 7 CV compared to the H(2p) peak near 4 cV. The high end of the c

distribution releases H-atoms with 10 eV kinet c energy. The low end of the distribution begins at about 1 eV. We have previously shown that the H(2p) distribution changes with electron impactenergy. A comparison of the results for H(3p) at 100 CV with those of Ogawa and co-workers is excellent. For example, their first measurement of H(3t) kinetic energy distribution from Hα line profile studies showed two kinds of kinetic energy distributions, an average kinetic energy of 7 eV associated with the fast group and an average kinetic energy of 0.3 eV attributed to the slow group. More detailed analysis of the Balmer series by Higo et al. followed. They measured the line profiles for Hα, Hβ and Hγ. At an electron impact energy of 100 Cv, the ranslational energy distributions had a fast peak a to 7-8 eV and a slow seak at -O eV.

The high kinetic energy fragments result from dissociation through a series of repulsive curves which involve doubly excited electron orbitals. These doubly excited stales have been described by Guberman .²⁰ The Q_1 Rydberg series of states consist of a $2p\sigma_u$ core orbital plus excited states of a symmetry. These repulsive states converge to the $^2\Sigma_u^+$ of $^{11}P_2^+$. The Q_2 Rydberg series of states consist of a $2p\pi_u$ core orbits] plus excited slates. These repulsive states converge to the $^2\Gamma_1$, of Π_2^+ . At 100 eV_1 mpact energy, both the Q_1 and Q_2 states can contribute to the approximately 4. Cv

of kinetic energy released to the pair of excited Ii--atoms at the peak of the 3p kinetic energy distribution in Fig. 3. However, The Q_1 state is the source of fas(H-atoms between 23 and 30 CV impact energies. A.5 The 10 west Q_1 ($^1\Sigma_g^{-1}(1)(2p\sigma_u)^2$) state crosses the Franck-Condon region at 23 eV. in our case, a curve crossing of this doubly excited state via homogeneous perturbation with the dissociating state ($1s\sigma_g$)(3t) (16.67eV dissociating energy) leads to the first group of fast H-atoms for n=3.

Ogawa and co-workers have carefully measure.d the central peak of the Hα line profile. They find the central peak of the Hα line profile to have a FWHM of 0.32Å at100 CV impact energy. They also find the central peak to be asymmetric due to fine structure. They find the same results as illustrated here from the point of view of line profile and kinetic energy distribution in Fig. 2 and Fig. 3, respectively, for the ratio of the fast to slow component H-atom intensities. The relative intensity of fast atoms increases with increasing principal quantum number. For H=2p we found that 31% of the atoms released in the dissociation processes are fast. 4.5 Integrating under the kinetic energy distribution curve for H=3p in fig. 3, we find that 47% of the atoms expelled in the dissociation process are fast. on a qualitative basis the line profile. compariso Is in Fig. 2 show the same results. If we take the central core FWHM reported by Ito et al. 1 and divide

by six, we would predict that the H Lβ central core should be 50 mÅ FWHM. On the other hand, our results suggest a FWH M of less than 30 mÅ. The difference may be ascribed to the lack of resolution in the Hα measurements to separate all the fine structure components. The complex line at 6562.8Å is composed of three multiplets at 6562.86 (2 p-3s), 6562.74 (2s-3p) and 6562.81 (2p-3d). Under higher resolution there are seven lines. The maximum separation is 120 mÅ and shows the difficulty of determining the slow atom energy (distribution from Hα line profiles.

DISCUSSION

We have measured the line profile of HL\$\beta\$ for the first time, and compared it to a higher resolution line profile of HL\$\alpha\$. The resolution was sufficient to determine the kinetic energy distribution function of fast H(3p) atoms from an analysis of the blue wing at 100 eV impact energy. Accurate analysis of the slow energy peak requires higher resolution studies of the line central peak. Preliminary results from our measurement indicate a line FWHM of less than 30 m\$\text{\A}\$ and a kinetic energy distribution with peak energy between O and 1 eV. The quantum yield of fast and slow atoms released in the various types of dissociation processes is 0.53 for slow atoms and 0.47 for fast atoms. A comparison of the fast kinetic

energy distribution for H(3p) from this experiment to that of H(3s,3p,3d) of Ogawa and co-workers are very similar. This result suggests that the three 1 lamultiplets have the same line profile at 100 CV electron impact energy.

Our direct measurement of the 11 LB cross section at 100 CV electron impact energy by two different methods arc in very good agreement with one another and yield an absolute cross section of 3.28 ± 0.80 x 10-19 cm². Duc to blending with nearby L& W bands, this measurement required a n estimate of the profile of the red wing. We assumed the line profile was symmetric, which causes about 10% uncertainty in the cross section. W c can extend the absolute cross section result at 100 CV to other energies by normalizing the low resolution H\alpha cross section results of Karolis and Harting⁷ from 0-105 CV and of Freundet al. 16 beyond 100 cV. This result is shown in Fig. 4. The excitation function indicates the four thresholds found by Karolis and Harting at 16, 26, 35 and 43 eV. Recently from high resolution studies of the excitation function of the Ila wing, Ogawa et al.³ found thresholds at 22-23 and 27 eV. in addition, we show in Fig. 4 the cross section for the entire blended feature of Fig. 1, inducting HLB and L & W features of Table 1. The cross section of the blended feature is 5.69 ± 0.80 x 1 0⁻¹⁰ cm² at 100 eV. The peak cross section for both excitation functions in Fig. 4 occur near 80 eV.

our previous indirect estimate of the HLβ cress section of 8.3 x 10- ¹⁹ cm² at 100 CV was based on the 3s, 3p, 3d excitation rates of Julien et al. ²1 and Glass-Maujean ²² However, the excitation rates were measured a t threshold (near 16.56 eV) and may change at higher energy. Additionally, these authors have measured the velocity distribution]] of fast and slow atoms, using measurements of anti-crossing signals between Zeeman sublevels. They have detected slow atoms with energies between 0.3 to 0.4 eV and fast atoms with energies of - 10 eV in good agreement with the results for fast atoms presented here. The Doppler shift ^{21,22} for the slow atoms corresponds to -30 mÅ, also in excellent agreement with our estimate.

We can also make an estimate of the contribution of 3p atoms to the H α cross section. The branching ratio, ω_{1s3p} , for is-3p emission is 0.881. The excitation cross section for 3p at 100 CV can be found to be $Q_{lp}/\omega_{1s3p}=3.72$ X 10^{-19} cm². On this basis we estimate that the 3p atoms contribute 40.0 \pm 10% of the total H α cross section of 9.3 x 10^{-19} cm². This fractional percentage indicate there is probably no preferential population of 3s, 3p, 3d sub-levels and the H α radiation is nearly the sum of the cross sections for 11(3s) and H(3d) dissociation. At 100 cV. Our results indicate that the

contribution to H α is 4.7% in agreement with earlier conclusions by Vroom and de Heer. Vroom and de Heer also indicate an upper limit to H(3p) dissociative cross section of 3.57 x 10^{-19} cm² at 50 eV. The cross section plot in Fig. 4 can be used to give the H(3p) cross section of 3.18 x 10-19 cm² at 50 Cv.

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Table 1 II₂ Emission Spectral Intensities near II Lyman-β Transition

Wavelength	Intensity ¹	Relative Intensity	Assignment ²
(A)	•	C
\			
1025.880	3.0490E-02	2.1256E-03	2(10, 5) P Werner
1025.886	4.6709E+00	3.2563E-01	1 (5, 3) Q Werner
1025.888	8.6408E-19	6.0240E-20	13(13, O) R Lyman
1025.895	2.3861E-04	1.6635E-05	4(11,11) Q D
1025.911	1.4344E+01	1.0000E+00	1 (3, 2) Q Werner
1025.918	8.3739E-08	5.8379E-09	8(2,5) QD
1025.922	1.0748E-07	7.4930E-09	6(11, 5) R Werner
1025.935	7.3617E+00	5.1323E-01	1 (6, O) P Lyman
1025.936	6.8840E-03	4.7992E-04	3(10, 5) R Werner
1025.957	5.9106E-O2	4.1206E-03	3 24, 4) P Lyman
1025.961	5.1620E-08	3.5987E-09	8 4, 2) Q Werner
1025.974	4.3545E-09	3.0358E-10	1 36, 5) P Lyman
1025.998	5.8953E-05	4.1099E-O6	6 5, 5) R B'
1026.016	2.2821E-10	1.5910E-31	1 35, 5) R Lyman
1026.019	8.7148E-02	6.0756E-03	1 14, 2) P Lyman
1026.072	1.3969E-13	9.7386E-15	10(19, 2) R Lyman
1026.079	3.51OOE-OI	2.4470E-02	3 (3, 6) Q D
1026.096	5.1721E-05	3.6058E-06	3(16,14) Q D
10?6.099	5.1928E-09	3.6202E-10	10(1, 3) PB'

¹ Effective intensities (unit: 10^{20} photon per H_2 molecule) 2 Transition is labelled by J''(v', v'') ΔJ . Lyman, Werner, B', and D refer to $2p\sigma$ $B^1\Sigma_u^+ \cdots X^1\Sigma_g^+$, $2p\pi$ $C^1\Pi_u \cdots X^1\Sigma_g^+$, $3p\sigma$ $B^{i-1}\Sigma_u^+ \cdots X^{-1}\Sigma_g^+$, and $3p\pi$ $D^1\Pi_u \cdots X^1\Sigma_g^+$ electronic transitions, respectively.

TABLE OF FIGURES

FIGURE 1. Overplot of experimental spectra: a) 100 eV HLβ line profile i n second order (open diamonds); b) 100 eV HLα line profile in third order (filled squares); c) zero order slit function of experimental apparatus scaled to second order (plus signs). The data statistics were better than 1% in a), b) and c).. The wavelength step size in second order was 4 mÅ a n c1 in third order was 2.667 mÅ. The operating conditions were established as follows: 1) background gas pressure of 2.3 x 10⁻⁴ torr and 2) electron beam current of 130 A. Peak signal was 4000 and 13000 counts in the 100 CV HLβ and HLα line profiles ,respectively, with background signals of under 100 counts.

FIGURE 2. Deconvolution of the 100 eV line profiles data of HL β (solid line) and 11 L α (dash line) of Fig. 1 along with a comparison to published data of H α line profiles.

FIGURE 3. Fast H(3p) and H(2p) atom kinetic energy distribution functions.

FIGURE 4. Estimated absolute cross section of H Lβ from published optical excitation function measurement of Hα. The excitation function measurements of Karolis and Harting⁷ shown as open diamonds from 0 - 100 CV and Freund et al. 16 shown as plus signs from 100-290 cV, are normalized to the 100 CV cross section of HLβ from this work. The cross section of the blended }1 Lβ & and 1. & W feature from this work is shown as a filled square.

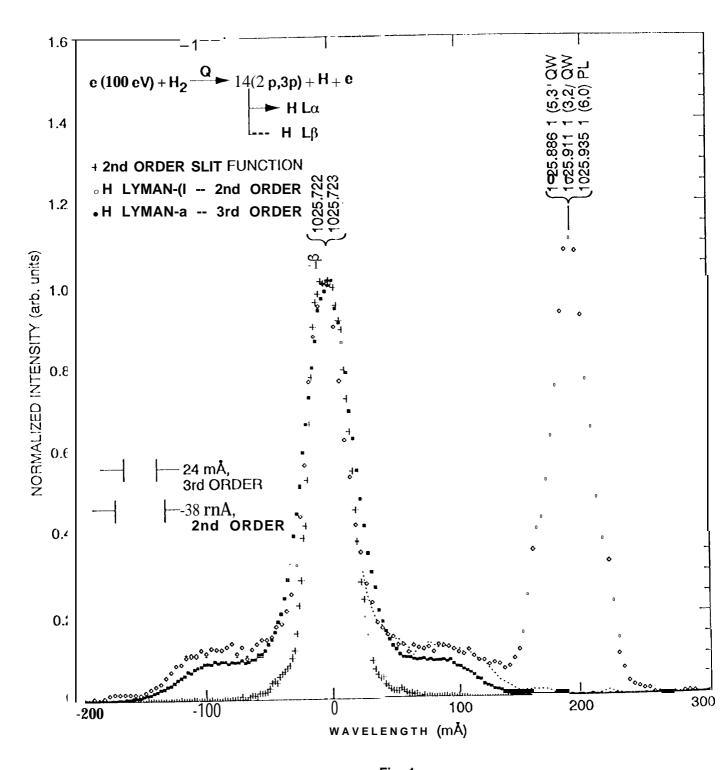
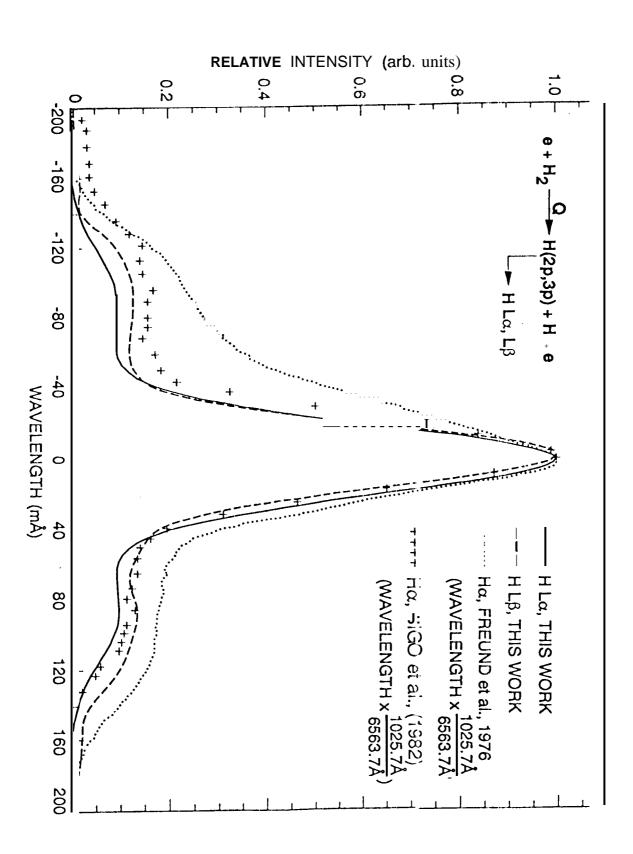


Fig. 1



-ig 2

